

Structural Characteristics and Dielectric Studies of $C_{21}H_{24}N_8 \cdot 2HCL$

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ABSTRACT

In the present work the structural and the dielectric studies for $C_{21}H_{24}N_8 \cdot 2HCL$ have been carried out in order to investigate the crystallographic and dielectric properties. Extensive experimentations have been performed to study the ferroelectric behaviour of $C_{21}H_{24}N_8 \cdot 2HCL$. The temperature and frequency dependence dielectric permittivity of $C_{21}H_{24}N_8 \cdot 2HCL$ ceramic has been studied in the temperature range of 26⁰C to 70⁰C at the frequencies, 1 kHz, 10 kHz, and 100 kHz. Its dielectric loss is also temperature dependent and it is very useful in conduction model. X-ray diffraction patterns indicate that the powder is crystalline in nature. In the present work, X-ray diffraction, dielectric and dielectric loss factors; studies have been carried out to make it suitable for device applications.

Keywords: Dielectric constant, ferroelectrics, dc conductivity.

INTRODUCTION

The dielectric constant and dielectric loss are important parameter for most applications of ferroelectric materials. Ferroelectricity is a common phenomenon and is exhibited by nearly all solids organic

or inorganic¹⁶. Barium titanate has already been studied as a high dielectric material, later in open publications it was concluded that the source of the high dielectric constant is due to its ferroelectric properties, ferroelectricity occurs in organic crystals polymers and also in liquid crystal⁹.

We have a relationship between the polarizability and the field (in linear response, for small electric field) which defines the dielectric susceptibility $\chi = P/E$. For an isotropic, linear dielectric, the polarization vector P is proportional and parallel to the applied field vector E . The electric flux density, or electric displacement, D is defined by (in cgs units)

$$D = E + 4\pi P = \epsilon E$$

Where ϵ is the static dielectric constant of the medium. From above eq. it follows that $\epsilon = 1 + 4\pi\chi$

where $\chi (= P/E)$ is the susceptibility. For isotropic dielectrics ϵ and χ are scalar quantities, which are dependent on the molecular properties of the dielectric^{8,13,14,15}. The dielectric constant is determined by the polarizability of the lattice.

The reversibility of their permanent polarization is one of the important feature of the ferroelectricity. Reversibility is due to the fact that the polar structure of ferroelectrics each can be derived from the non polar crystal structure by high deformation. This reversibility of permanent polarization leads to a non linear dielectric behavior⁴.

In general a ferroelectric crystal consist of domain which are small regions of homogenous polarization. The direction of polarization differs in the various domains. The study of domain formation is important for controlling and modulating the materials property⁹ as the performance of ferroelectric material is essentially related to their microstructure in particular domain structure¹².

The properties of ferroelectric materials highly depend on the process they

are prepared. Therefore, during the synthesis of ferroelectric materials the composition homogeneity is one of the most important factors to be maintained in the specimen^{6,7,12,18}. In ferroelectric materials the other important parameters are the dielectric constant, hysteresis phenomenon and microstructure which characteristics define the properties of ferroelectric materials under investigations¹. Grain size is another important factor which determines the properties as dielectric constant, phase transition temperature (T_c), polarization, piezoelectric and pyroelectric co-efficient of ferroelectric ceramics^{3,10,11,17}. It is thus imperative to discuss these properties. Mostly, highly dense ferroelectric materials are required for various applications because full densification of ferroelectric materials ensures to achieve the maximized performance. The dielectric constant of ferroelectric ceramics usually increases with increasing density. Generally, the densities of ferroelectric ceramics increase with increasing sintering temperature. However there is temperature limit for some ferroelectric materials. High temperature also leads to abnormal grain growth which is harmful to the performance for most ferroelectric ceramics.

EXPERIMENTAL

The $C_{21}H_{24}N_8 \cdot 2HCl$ have been procured in the powder form from Fluka (Sigma Aldrich Chemicals Pvt. Ltd., New Delhi). The powder has been kept in enclosed container before using them for experimentation.

$C_{21}H_{24}N_8 \cdot 2HCl$ powder were taken and compressed on glass slides for x-ray diffraction studies. The XRD studies have

been carried out on a Rizaku 18 KW rotating powder X-ray diffractometer operated at 5 KVA. The scan speed was maintained to 2° /min and the XRD patterns were collected for 2θ varying 20 to 70 degree.

For the dielectric studies the powder was taken into a mortar piston. The powder was then crunched and mixed properly. The so obtained fine powders of $C_{21}H_{24}N_8 \cdot 2HCL$ were used to prepare circular pellets.

The edges of pellets were cleaned by emery paper in order to remove Fe particles. The circular pellets were then electroded with silver paint in order to make the surface conducting². The electrode circular disc was put into oven for complete dryness. The sample of electroded $C_{21}H_{24}N_8 \cdot 2HCL$ was

then put into small furnace which contains thermocouple and connected to LCR meter and a variac. The temperature was controlled by using a PID temperature controlled system. All the measurements were taken at a constant heating rate of $1^\circ C/min$.

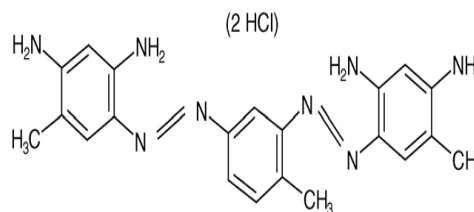


Figure-1. The structural formula of the $C_{21}H_{24}N_8 \cdot 2HCL$

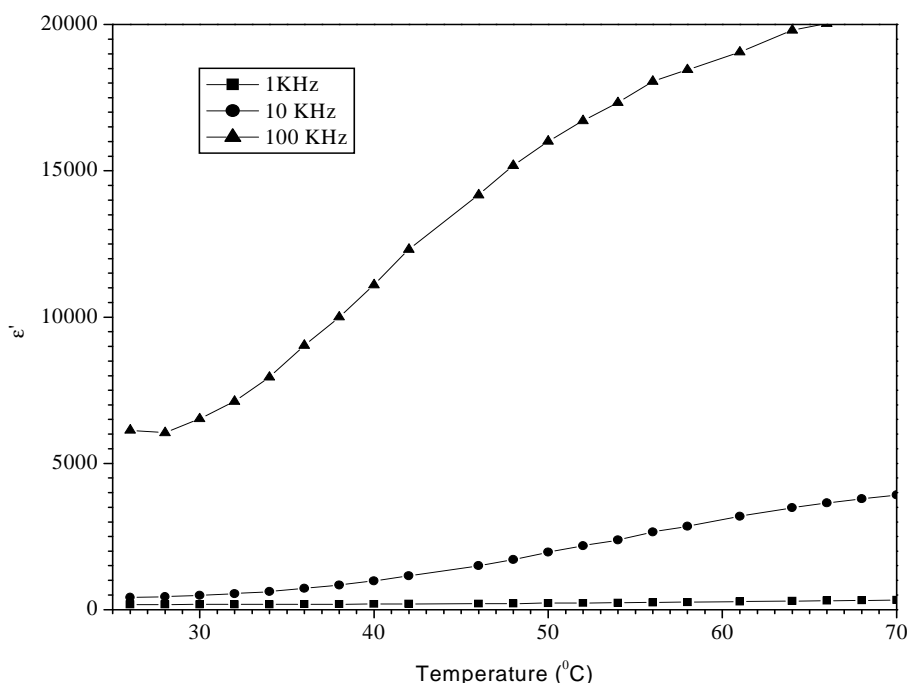


Figure 2- Temperature dependent dielectric constant (real part) of $C_{21}H_{24}N_8 \cdot 2HCL$

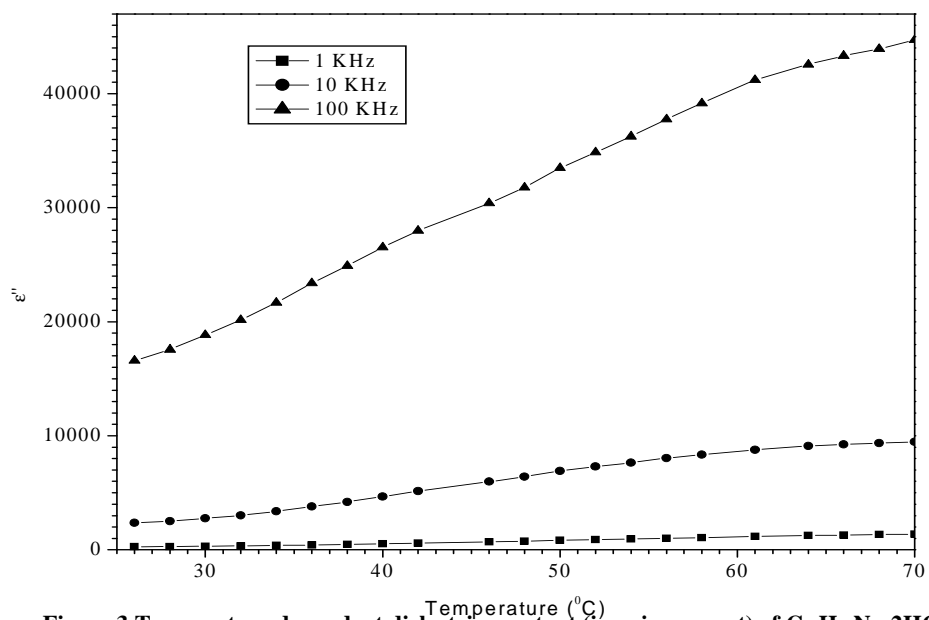


Figure 3 Temperature dependent dielectric constant (imaginary part) of $C_{21}H_{24}N_8 \cdot 2HCL$

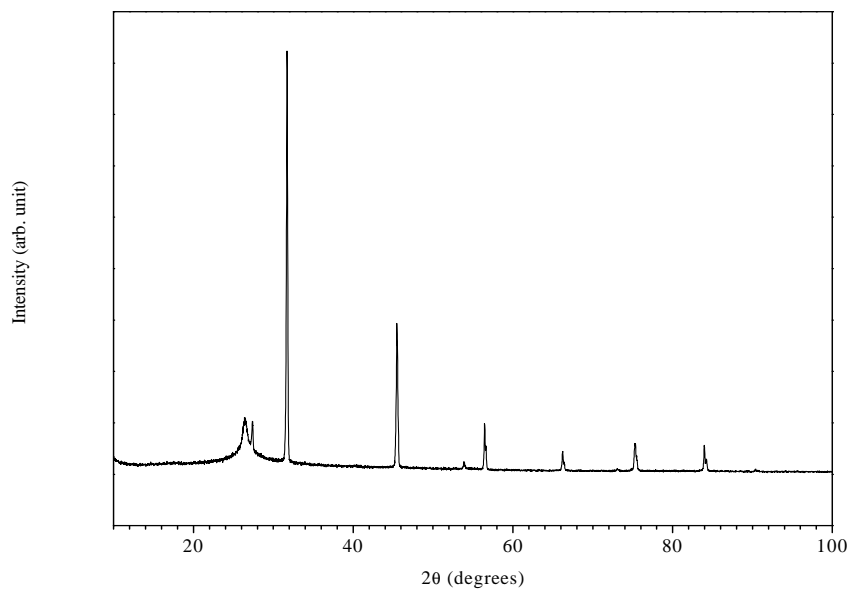


Figure 4 Powder XRD pattern of $C_{21}H_{24}N_8 \cdot 2HCL$

RESULTS AND DISCUSSION:

The temperature and frequency dependent real and imaginary parts of dielectric measurement for $C_{21}H_{24}N_8 \cdot 2HCL$ have been depicted in figure 2 & 3 respectively where as the room temperature dielectric constant with varying frequency is shown in table 1. It can be inferred from the table that the room temperature dielectric constant of $C_{21}H_{24}N_8 \cdot 2HCL$ is around 6000 at 100 KHZ where as the values at 1 & 10 KHZ are less than 100. The highest dielectric constant value at 100 KHZ reveals that interference of wave damping is restricted at this frequency where as at 1 KHZ and 10 KHZ there is a interference if frequency factor to reduce the value of dielectric constant drastically. The temperature dependence value of dielectric constant as depicted in figure (2) exhibits that increasing temperature from room temperature to 70°C the dielectric constant increases. Increase in dielectric constant at higher temperature can be attributed to the increase in dc conductivity with temperature as observed in Ba_2BiSbO_6 , $BaSrBiSbO_6$ and several other compounds^{5,16,19}. It can be seen from figure that upto 62°C there is a linear growth of dielectric constant with temperature.

The XRD of $C_{21}H_{24}N_8 \cdot 2HCL$ have been shown in figure (4). It is evident from the diffractogram that the $C_{21}H_{24}N_8 \cdot 2HCL$ powder is crystalline in nature as reported earlier by several workers. It is also evident from fig. that the structure of $C_{21}H_{24}N_8 \cdot 2HCL$ is tetragonal where $a = b \neq c$ and α, β, γ is 90° . In the patterns there is no evidence of super lattice or **purochore** phase which suggest that $C_{21}H_{24}N_8 \cdot 2HCL$ is highly pure in nature and resembles a perovskite structure as reported earlier.

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